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(*E*)-*N*′-(2-Chlorobenzylidene)-2-methoxybenzohydrazide

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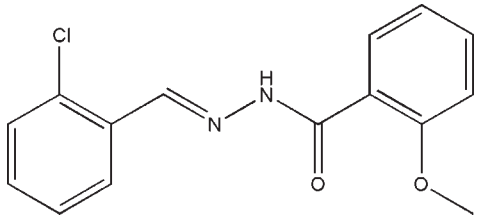
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 16.1.

The molecule of the title compound, $C_{15}H_{13}ClN_2O_2$, displays an *E* configuration about the C=N bond. The dihedral angle between the two benzene rings is 77.1 (2)°. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds, forming chains running along the *b* axis.

Related literature

For examples of the crystal structures of hydrazone compounds, see: Mohd Lair *et al.* (2009); Fun *et al.* (2008); Li & Ban (2009); Zhu *et al.* (2009); Yang (2007); You *et al.* (2008). For the hydrazone compounds we have reported previously, see: Qu *et al.* (2008); Yang *et al.* (2008), Cao & Lu (2009*a*,*b*), Qu & Cao (2009), Cao & Wang (2009).



Experimental

Crystal data

$C_{15}H_{13}ClN_2O_2$
M_r = 288.72
Orthorhombic, *Pbca*
a = 12.808 (2) Å
b = 9.719 (2) Å
c = 21.882 (1) Å
V = 2723.9 (7) Å^3
Z = 8
Mo *K*α radiation
μ = 0.28 mm^{-1}
T = 298 K
0.30 × 0.27 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.920, T_{max} = 0.928
15666 measured reflections
2977 independent reflections
2317 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
2977 reflections
185 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.895 (10)	2.005 (11)	2.8791 (16)	165 (2)

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The Vital Foundation of Ankang University (project No. 2008AKXY012) and the Special Scientific Research Foundation of the Education Office of Shanxi Province (Project No. 02JK202) are gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2366).

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supporting information

Acta Cryst. (2009). E**65**, o2650 [https://doi.org/10.1107/S1600536809039725]

(*E*)-*N*′-(2-Chlorobenzylidene)-2-methoxybenzohydrazide

Guo-Biao Cao

S1. Comment

Study on the crystal structures of hydrazone derivatives is an interesting topic in structural chemistry. Recently, the crystal structures of a number of hydrazone compounds have been reported (Mohd Lair *et al.*, 2009; Fun *et al.*, 2008; Li & Ban, 2009; Zhu *et al.*, 2009; Yang, 2007; You *et al.*, 2008). As a continuation of our work in this area (Qu *et al.*, 2008; Yang *et al.*, 2008; Cao & Lu, 2009a,b; Qu & Cao, 2009; Cao & Wang, 2009), the title new hydrazone compound, derived from the reaction of 2-chlorobenzaldehyde with an equimolar quantity of 2-methoxybenzohydrazide, is reported.

The molecule of the title compound (Fig. 1) displays an *E* configuration about the C═N bond. The dihedral angle between the two benzene rings is 77.1 (2)°. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1) to form chains running along the *b* axis (Fig. 2).

S2. Experimental

The title compound was prepared by refluxing 2-chlorobenzaldehyde (0.1 mmol, 14.0 mg) with 2-methoxybenzohydrazide (0.1 mmol, 16.6 mg) in methanol (20 ml). Colourless block-like crystals were formed by slow evaporation of the solution in air.

S3. Refinement

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93-0.96 Å, and with U_{iso}(H) set at 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

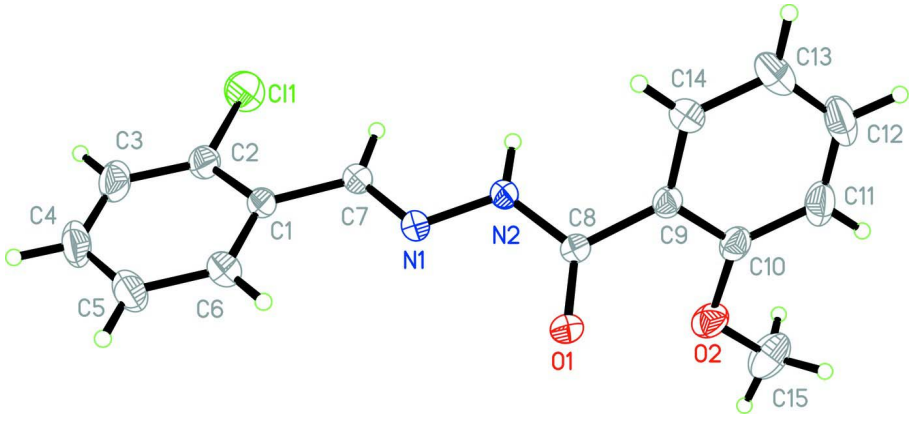

Figure 1

The molecular structure of the title compound with ellipsoids drawn at the 30% probability level.

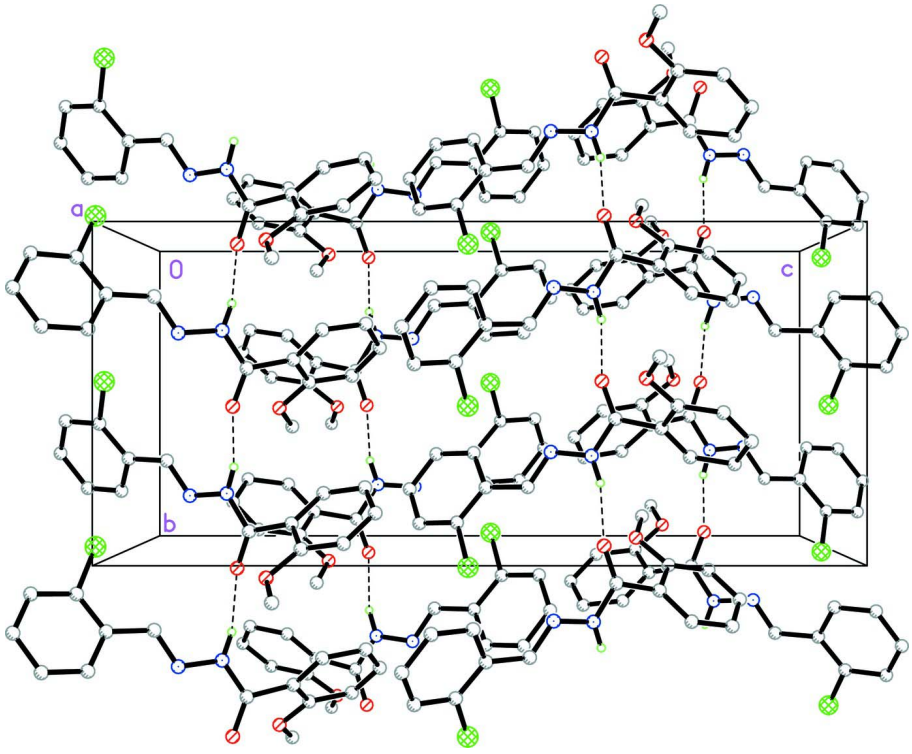

Figure 2

The molecular packing of the title compound, viewed along the *a* axis. Hydrogen bonds are drawn as dashed lines.

(*E*)-*N*′-(2-Chlorobenzylidene)-2-methoxybenzohydrazide

Crystal data

$C_{15}H_{13}ClN_2O_2$
$M_r = 288.72$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.808$ (2) Å
$b = 9.719$ (2) Å
$c = 21.882$ (1) Å
$V = 2723.9$ (7) Å^3
$Z = 8$
$F(000) = 1200$
$D_x = 1.408$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4172 reflections
$\theta = 2.4$–$26.7°$
$\mu = 0.28$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.27 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.920$, $T_{max} = 0.928$
15666 measured reflections
2977 independent reflections
2317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.9°$
$h = -16 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.103$
$S = 1.05$
2977 reflections
185 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.9256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.69237 (5)	1.03716 (5)	0.48396 (2)	0.07052 (19)
N1	0.65156 (10)	0.68177 (13)	0.59858 (5)	0.0376 (3)
N2	0.70523 (10)	0.69184 (13)	0.65323 (6)	0.0368 (3)
O1	0.70476 (9)	0.46137 (10)	0.66748 (5)	0.0429 (3)
O2	0.91235 (9)	0.45442 (12)	0.71914 (6)	0.0519 (3)
C1	0.59496 (13)	0.79503 (16)	0.50823 (7)	0.0397 (4)
C2	0.60523 (14)	0.90535 (19)	0.46817 (7)	0.0473 (4)
C3	0.54802 (17)	0.9123 (2)	0.41464 (8)	0.0630 (5)
H3	0.5550	0.9877	0.3888	0.076*
C4	0.48113 (17)	0.8075 (3)	0.39982 (8)	0.0691 (6)
H4	0.4425	0.8124	0.3639	0.083*
C5	0.47062 (15)	0.6950 (2)	0.43767 (8)	0.0616 (5)
H5	0.4259	0.6234	0.4271	0.074*
C6	0.52691 (14)	0.68944 (19)	0.49135 (8)	0.0501 (4)
H6	0.5194	0.6136	0.5169	0.060*
C7	0.65157 (13)	0.79086 (16)	0.56644 (7)	0.0399 (4)
H7	0.6876	0.8682	0.5799	0.048*
C8	0.72722 (11)	0.57716 (15)	0.68513 (6)	0.0328 (3)
C9	0.77783 (12)	0.60482 (15)	0.74570 (7)	0.0363 (3)
C10	0.86873 (13)	0.53644 (16)	0.76282 (7)	0.0429 (4)
C11	0.90966 (17)	0.5564 (2)	0.82074 (9)	0.0602 (5)
H11	0.9706	0.5113	0.8323	0.072*
C12	0.85998 (19)	0.6431 (3)	0.86112 (9)	0.0716 (6)
H12	0.8868	0.6538	0.9003	0.086*

C13	0.77176 (17)	0.7140 (2)	0.84470 (8)	0.0634 (5)
H13	0.7399	0.7742	0.8720	0.076*
C14	0.73121 (14)	0.69436 (17)	0.78697 (7)	0.0453 (4)
H14	0.6714	0.7420	0.7754	0.054*
C15	1.01129 (16)	0.3943 (3)	0.73206 (11)	0.0753 (7)
H15A	1.0616	0.4657	0.7393	0.113*
H15B	1.0332	0.3395	0.6979	0.113*
H15C	1.0058	0.3372	0.7677	0.113*
H2	0.7296 (17)	0.7743 (14)	0.6645 (9)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1003 (4)	0.0546 (3)	0.0567 (3)	−0.0134 (3)	−0.0006 (3)	0.0130 (2)
N1	0.0449 (7)	0.0357 (7)	0.0323 (6)	0.0034 (6)	−0.0073 (5)	−0.0016 (5)
N2	0.0478 (7)	0.0295 (6)	0.0330 (6)	−0.0012 (5)	−0.0091 (5)	0.0000 (5)
O1	0.0548 (7)	0.0287 (6)	0.0451 (6)	0.0017 (5)	−0.0090 (5)	−0.0018 (5)
O2	0.0435 (7)	0.0469 (7)	0.0654 (8)	0.0123 (5)	−0.0045 (6)	0.0001 (6)
C1	0.0478 (9)	0.0403 (8)	0.0311 (7)	0.0094 (7)	−0.0030 (6)	−0.0032 (6)
C2	0.0583 (10)	0.0487 (10)	0.0349 (8)	0.0099 (8)	0.0001 (7)	0.0014 (7)
C3	0.0777 (14)	0.0747 (13)	0.0367 (9)	0.0216 (12)	−0.0060 (9)	0.0072 (9)
C4	0.0683 (13)	0.1022 (17)	0.0369 (9)	0.0257 (13)	−0.0174 (9)	−0.0083 (10)
C5	0.0551 (11)	0.0802 (14)	0.0496 (10)	0.0067 (10)	−0.0126 (9)	−0.0189 (10)
C6	0.0569 (11)	0.0512 (10)	0.0423 (9)	0.0029 (8)	−0.0069 (8)	−0.0070 (8)
C7	0.0499 (9)	0.0343 (8)	0.0354 (8)	0.0011 (7)	−0.0064 (7)	−0.0013 (6)
C8	0.0341 (8)	0.0298 (7)	0.0344 (7)	0.0018 (6)	−0.0001 (6)	0.0000 (6)
C9	0.0416 (8)	0.0313 (7)	0.0360 (7)	−0.0032 (6)	−0.0028 (6)	0.0051 (6)
C10	0.0458 (9)	0.0358 (8)	0.0470 (9)	−0.0043 (7)	−0.0057 (7)	0.0096 (7)
C11	0.0641 (12)	0.0619 (12)	0.0547 (11)	−0.0081 (10)	−0.0251 (9)	0.0154 (9)
C12	0.0886 (16)	0.0872 (16)	0.0389 (10)	−0.0188 (13)	−0.0197 (10)	0.0042 (10)
C13	0.0757 (14)	0.0748 (14)	0.0397 (9)	−0.0136 (11)	0.0018 (9)	−0.0127 (9)
C14	0.0503 (10)	0.0452 (9)	0.0406 (8)	0.0002 (8)	−0.0008 (7)	−0.0055 (7)
C15	0.0493 (11)	0.0764 (15)	0.1003 (17)	0.0188 (11)	0.0003 (11)	0.0219 (13)

Geometric parameters (Å, º)

Cl1—C2	1.734 (2)	C5—H5	0.9300
N1—C7	1.2723 (19)	C6—H6	0.9300
N1—N2	1.3830 (17)	C7—H7	0.9300
N2—C8	1.3449 (18)	C8—C9	1.500 (2)
N2—H2	0.895 (10)	C9—C14	1.389 (2)
O1—C8	1.2241 (17)	C9—C10	1.392 (2)
O2—C10	1.364 (2)	C10—C11	1.385 (2)
O2—C15	1.424 (2)	C11—C12	1.377 (3)
C1—C2	1.391 (2)	C11—H11	0.9300
C1—C6	1.396 (2)	C12—C13	1.371 (3)
C1—C7	1.466 (2)	C12—H12	0.9300
C2—C3	1.383 (2)	C13—C14	1.379 (2)

C3—C4	1.369 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.379 (3)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.379 (2)	C15—H15C	0.9600

C7—N1—N2	114.77 (13)	O1—C8—C9	123.04 (13)
C8—N2—N1	119.62 (12)	N2—C8—C9	113.62 (12)
C8—N2—H2	121.7 (14)	C14—C9—C10	118.93 (15)
N1—N2—H2	118.4 (14)	C14—C9—C8	120.07 (14)
C10—O2—C15	117.73 (16)	C10—C9—C8	120.91 (14)
C2—C1—C6	117.31 (15)	O2—C10—C11	124.60 (16)
C2—C1—C7	121.47 (15)	O2—C10—C9	115.66 (14)
C6—C1—C7	121.21 (15)	C11—C10—C9	119.73 (17)
C3—C2—C1	121.39 (18)	C12—C11—C10	119.87 (19)
C3—C2—Cl1	118.28 (15)	C12—C11—H11	120.1
C1—C2—Cl1	120.32 (13)	C10—C11—H11	120.1
C4—C3—C2	119.72 (19)	C13—C12—C11	121.35 (17)
C4—C3—H3	120.1	C13—C12—H12	119.3
C2—C3—H3	120.1	C11—C12—H12	119.3
C3—C4—C5	120.57 (17)	C12—C13—C14	118.72 (19)
C3—C4—H4	119.7	C12—C13—H13	120.6
C5—C4—H4	119.7	C14—C13—H13	120.6
C4—C5—C6	119.45 (19)	C13—C14—C9	121.37 (17)
C4—C5—H5	120.3	C13—C14—H14	119.3
C6—C5—H5	120.3	C9—C14—H14	119.3
C5—C6—C1	121.52 (18)	O2—C15—H15A	109.5
C5—C6—H6	119.2	O2—C15—H15B	109.5
C1—C6—H6	119.2	H15A—C15—H15B	109.5
N1—C7—C1	120.21 (14)	O2—C15—H15C	109.5
N1—C7—H7	119.9	H15A—C15—H15C	109.5
C1—C7—H7	119.9	H15B—C15—H15C	109.5
O1—C8—N2	123.30 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.90 (1)	2.01 (1)	2.8791 (16)	165 (2)

Symmetry code: (i) −*x*+3/2, *y*+1/2, *z*.